Enrollment ID: _____

NAVRACHANA UNIVERSITY
a UGC recognized University

School: School of Science
Program: M.Sc. in Chemistry
Year: 1st **Semester:** I
Examination: End Sem Examination
Examination year: December - 2022

Course Code: CH132 **Course Name:** Quantum Mechanics & Group Theory

Date: 12/12/2022
Time: 11:30 am to 1:30 pm

Total Marks: 40
Total Pages: 2

Instructions:

- *All Sections are compulsory.*
- *Please read the questions carefully and answer accordingly.*
- *Draw a neat and labeled diagram wherever necessary.*

		Co	BT
Q.1. Answer in details. (Any four, each carry 5 marks) i. Derive the term symbols for d^1 to d^5 system. ii. Calculate the Raman and IR active band for $POCl_3$ using appropriate character table. (no need to write character table in answer sheet) iii. Find the wavelength of radiation emitted by an atom when an excited electron of it drops from quantum level n=2 to the level n=1 consider an electron within an atom size 2A°. iv. Derive the energy equation for "zero point energy". v. Explain how external magnetic field effect the splitting of H atom spectral line. vi. Justify that, p-orbitals follow all the symmetry operations for C_{2v} point group.	**20**		**BT1** **BT2** **BT3** **BT4** **BT5**
Q.2. Answer in brief. (Any Five, each carry 02 marks) i. Write all symmetry elements and point group for the (a) Trans-EthaneBr_2Cl_2 (b) EtheneBrCl ii. Write about limitations of wave functions. iii. What mean by Stark Effect, write in detail. iv. What means by subgroup, explain it by proper example. v. Write about the equation which shows relationship between magnetic dipole moment μ and the exterior magnetic field B. Define the each terms. vi. Write all the equations for an observable that is represented in classical physics by a function Q(x,p), the corresponding operatore is $Q(\hat{x}, \hat{p})$.	**10**	**CO1** **CO2** **CO3** **CO4** **CO5** **CO6**	**BT1** **BT2** **BT3** **BT4**
Q.3. Answer in short	**05**		

i. The Molecule of CO_2 belongs which point group?			BT1
ii. Acetylene belongs which point group?			BT2
iii. Hydrogen cyanide belongs to which point group?			BT3
iv. The dual nature of wave was proposed whom.			BT4
v. What Bohr's atomic model explain.			
Q.4. Write True or False and Justify	05		BT1
i. quadratic Stark effect is not arises due to a dipole moment that arises from a naturally occurring non-symmetric distribution of electrical charge.			BT2
ii. Anomalous Zeeman effect is caused by the interaction with the orbital magnetic moment.			BT3
iii. $V = -\frac{Z}{r1} + \sum_{j=1} 1/r1j$, here Z represent the atomic number of atom.			BT4
iv. $\hat{H} = [-1/2\sum_i V_i^2 - \sum_i \frac{\bar{Z}}{r_i}] + 1/2\sum_{i\neq j} 1/r_{ij}$, Here second term represent the sum of single electron.			
v. $[Co(NH_3)_5]^{2+}$ does not have point of inversion.			

-------End of Question Paper--------

Character Tables

D_{3h}	E	$2C_3$ (z)	$3C'_2$	σ_h (xy)	$2S_3$	$3\sigma_v$	Linear functions, rotations	Quadratic functions
A'_1	+1	+1	+1	+1	+1	+1	-	x^2+y^2, z^2
A'_2	+1	+1	-1	+1	+1	-1	R_z	-
E'	+2	-1	0	+2	-1	0	(x, y)	(x^2-y^2, xy)
A''_1	+1	+1	+1	-1	-1	-1	-	-
A''_2	+1	+1	-1	-1	-1	+1	z	-
E''	+2	-1	0	-2	+1	0	(R_x, R_y)	(xz, yz)

C_{2v}	E	C_2 (z)	σ_v(xz)	σ_v(yz)	Linear functions, rotations	Quadratic functions
A_1	+1	+1	+1	+1	z	x^2, y^2, z^2
A_2	+1	+1	-1	-1	R_z	xy
B_1	+1	-1	+1	-1	x, R_y	xz
B_2	+1	-1	-1	+1	y, R_x	yz

C_{3v}	E	$2C_3$ (z)	$3\sigma_v$	Linear functions, rotations	Quadratic functions
A_1	+1	+1	+1	z	x^2+y^2, z^2
A_2	+1	+1	-1	R_z	-
E	+2	-1	0	(x, y) (R_x, R_y)	(x^2-y^2, xy) (xz, yz)

T_d	E	$8C_3$	$3C_2$	$6S_4$	$6\sigma_d$	Linear functions, rotations	Quadratic functions
A_1	+1	+1	+1	+1	+1	-	$x^2+y^2+z^2$
A_2	+1	+1	+1	-1	-1	-	-
E	+2	-1	+2	0	0	-	$(2z^2-x^2-y^2, x^2-y^2)$
T_1	+3	0	-1	+1	-1	(R_x, R_y, R_z)	-
T_2	+3	0	-1	-1	+1	(x, y, z)	(xy, xz, yz)

D_{4h}	E	$2C_4(z)$	C_2	$2C'_2$	$2C''_2$	i	$2S_4$	σ_h	$2\sigma_v$	$2\sigma_d$	Linear functions, rotations	Quadratic functions
A_{1g}	+1	+1	+1	+1	+1	+1	+1	+1	+1	+1	-	x^2+y^2, z^2
A_{2g}	+1	+1	+1	-1	-1	+1	+1	+1	-1	-1	R_z	-
B_{1g}	+1	-1	+1	+1	-1	+1	-1	+1	+1	-1	-	x^2-y^2
B_{2g}	+1	-1	+1	-1	+1	+1	-1	+1	-1	+1	-	xy
E_g	+2	0	-2	0	0	+2	0	-2	0	0	(R_x, R_y)	(xz, yz)
A_{1u}	+1	+1	+1	+1	+1	-1	-1	-1	-1	-1	-	-
A_{2u}	+1	+1	+1	-1	-1	-1	-1	-1	+1	+1	z	-
B_{1u}	+1	-1	+1	+1	-1	-1	+1	-1	-1	+1	-	-
B_{2u}	+1	-1	+1	-1	+1	-1	+1	-1	+1	-1	-	-
E_u	+2	0	-2	0	0	-2	0	+2	0	0	(x, y)	-

C_{2h}	E	C_2	I	σ_h	Linear functions, rotations	Quadratic functions
A_g	1	1	1	1	R_z	X^2, y^2, z^2, xy
B_g	1	-1	1	-1	R_x, R_y	xz, yz
A_u	1	1	-1	-1	Z	-
B_u	1	-1	-1	1	X,Y	-

O_h	E	$8C_3$	$6C_2$	$6C_4$	$3C_2=(C_4)^2$	i	$6S_4$	$8S_6$	$3\sigma_h$	$6\sigma_d$	Linear functions, rotations	Quadratic functions
A_{1g}	+1	+1	+1	+1	+1	+1	+1	+1	+1	+1	-	$x^2+y^2+z^2$
A_{2g}	+1	+1	-1	-1	+1	+1	-1	+1	+1	-1	-	-
E_g	+2	-1	0	0	+2	+2	0	-1	+2	0	-	$(2z^2-x^2-y^2, x^2-y^2)$
T_{1g}	+3	0	-1	+1	-1	+3	+1	0	-1	-1	(R_x, R_y, R_z)	-
T_{2g}	+3	0	+1	-1	-1	+3	-1	0	-1	+1	-	(xz, yz, xy)
A_{1u}	+1	+1	+1	+1	+1	-1	-1	-1	-1	-1	-	-
A_{2u}	+1	+1	-1	-1	+1	-1	+1	-1	-1	+1	-	-
E_u	+2	-1	0	0	+2	-2	0	+1	-2	0	-	-
T_{1u}	+3	0	-1	+1	-1	-3	-1	0	+1	+1	(x, y, z)	-
T_{2u}	+3	0	+1	-1	-1	-3	+1	0	+1	-1	-	-

D_{2d}	E	$2S_4$	$C_2(z)$	$2C'_2$	$2\sigma_d$	Linear functions, rotations	Quadratic functions
A_1	+1	+1	+1	+1	+1	-	x^2+y^2, z^2
A_2	+1	+1	+1	-1	-1	R_z	-
B_1	+1	-1	+1	+1	-1	-	x^2-y^2
B_2	+1	-1	+1	-1	+1	z	xy
E	+2	0	-2	0	0	(x, y) (R_x, R_y)	(xz, yz)

---------End of Question Paper---------